

Direct Observations of the Real Structures of Crystals of Some Tetrahedrally Close-Packed Alloys

A High Resolution Electron
Microscopy Study

IMAGES and LEGENDS

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Lund 1984



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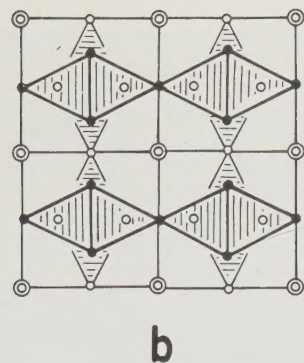
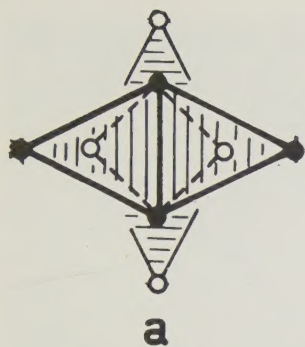


Fig 1a. Tetraederstern (TS). This polyhedron is constructed by five non-centered, slightly distorted tetrahedra (the central one is outlined with dashed lines). Filled and open circles represent atoms in two different planes.

Fig 1b. The A15 structure (β -W, Cr_3Si), constructed by TS's sharing corners. Filled, open and double circles represent atoms at 0, $1/2$ and $1/4$ and $3/4$ respectively.

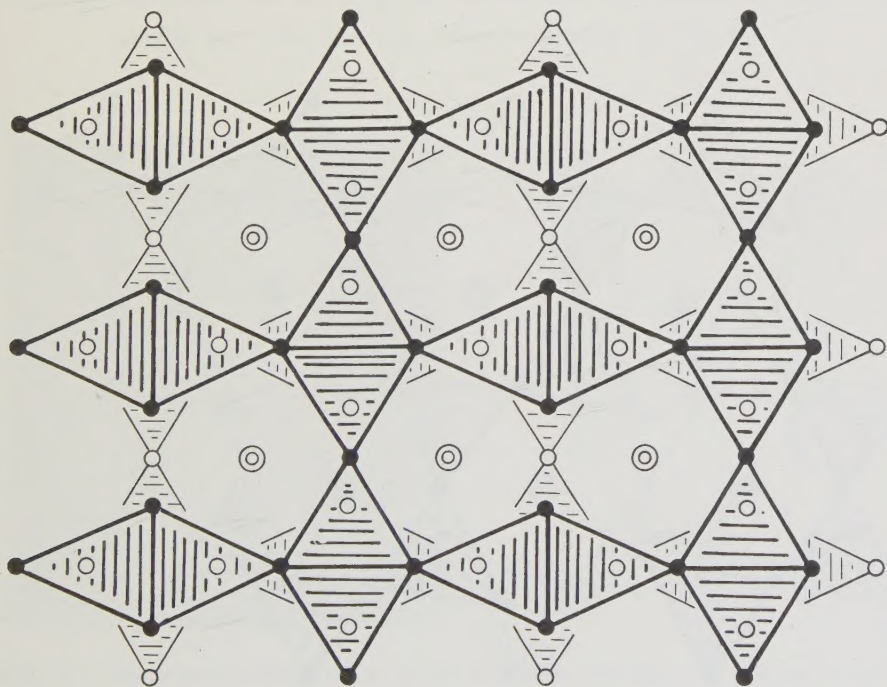


Fig 2. The real structure of Zr_4Al_3 viewed along $[110]$. The ideal arrangement can be derived from the A15 structure with regular crystallographic shear (CS) operations in one direction. The TS's will hence become corner- and edgesharing.

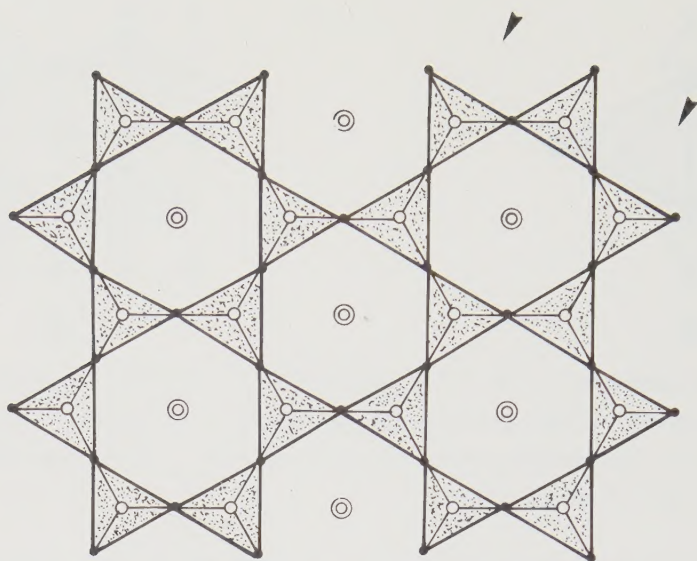


Fig 3. The structure of Zr_4Al_3 projected along the c -axis. Regular CS operations in the direction of the arrows gives the MgCu_2 -structure.

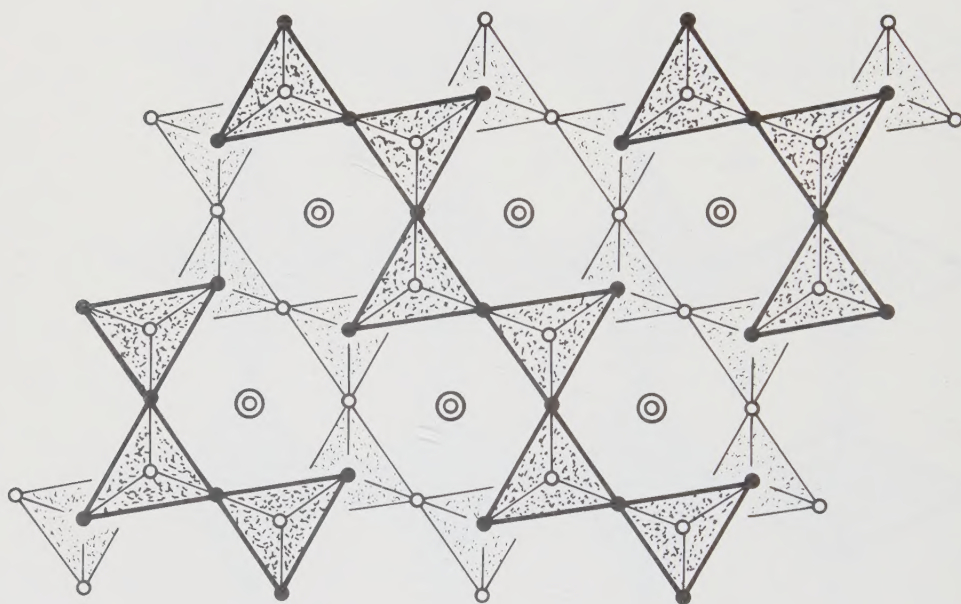


Fig 4. The structure of MgCu_2 projected along $[1\bar{1}0]$. The CS operation described in Fig 3 creates atomic positions with CN 16 along the shared edges of the trigonal bi-pyramids.

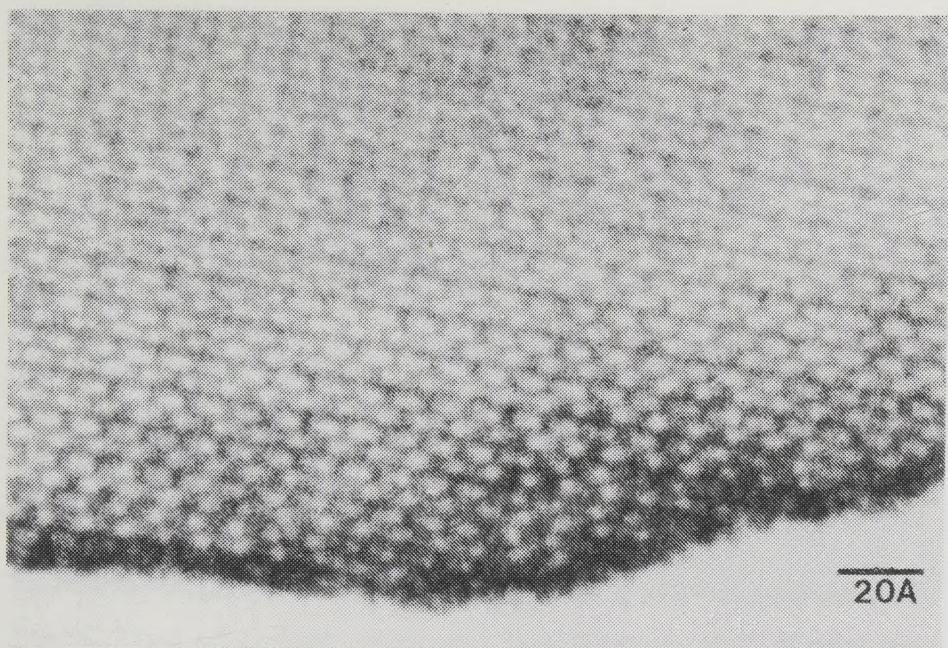


Fig 5a. Lattice image of a Fe-Mo σ -phase crystal. The white dots correspond to the positions of the atoms encircled in Fig 5c.

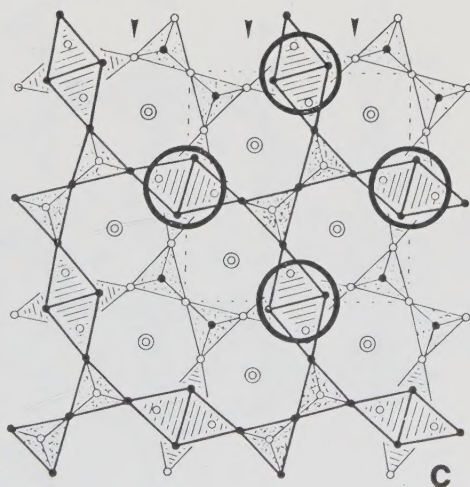
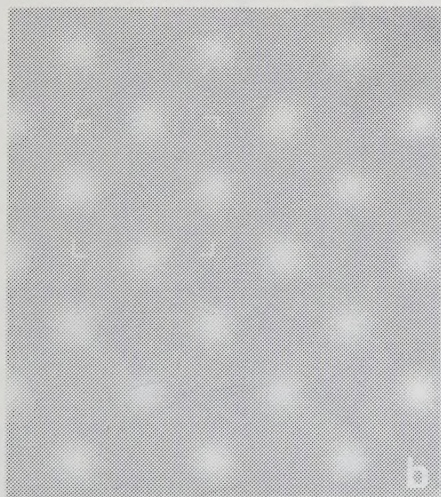


Fig 5b. Calculated image of a Fe-Mo σ -phase. Corners of the unit cell are indicated (NSLICE = 6, $\Delta f = -900$ Å).

Fig 5c. Structural drawing of the σ -phase along the c -axis. Circles include atomic sites with predominantly Mo-atoms. Arrows show possible planes for chemical twinning.

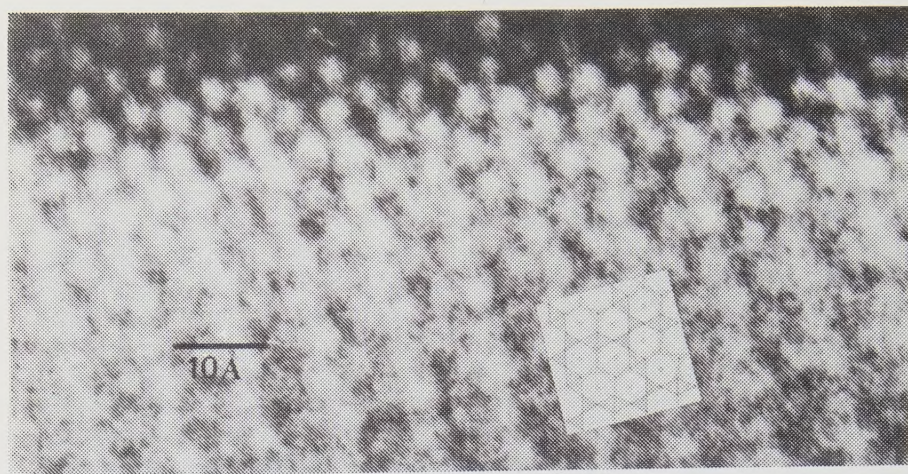


Fig 5d. Crystal Structure Image (CSI) of a σ -phase crystal of mainly Fe and Cr. The white dots represent the positions of the atoms centering the hexagonal anti-prisms (double circles in Fig 5c).

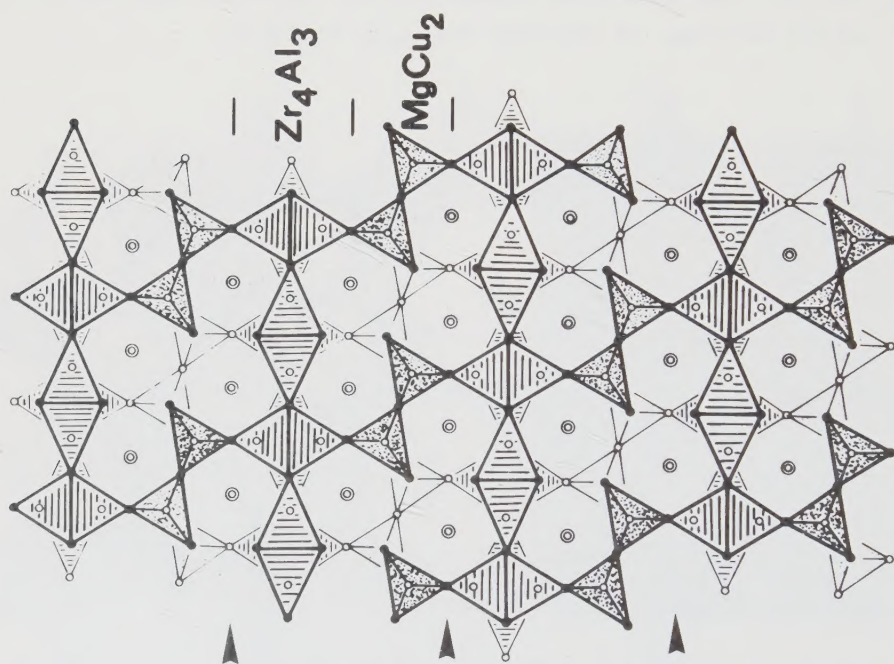


Fig 6a. Structural drawing of the μ -phase. Regular twin operations along arrows will give the structure of K_7Cs_6 . The structure is an intergrowth between slabs with Zr_4Al_3 - and $MgCu_2$ -structures.

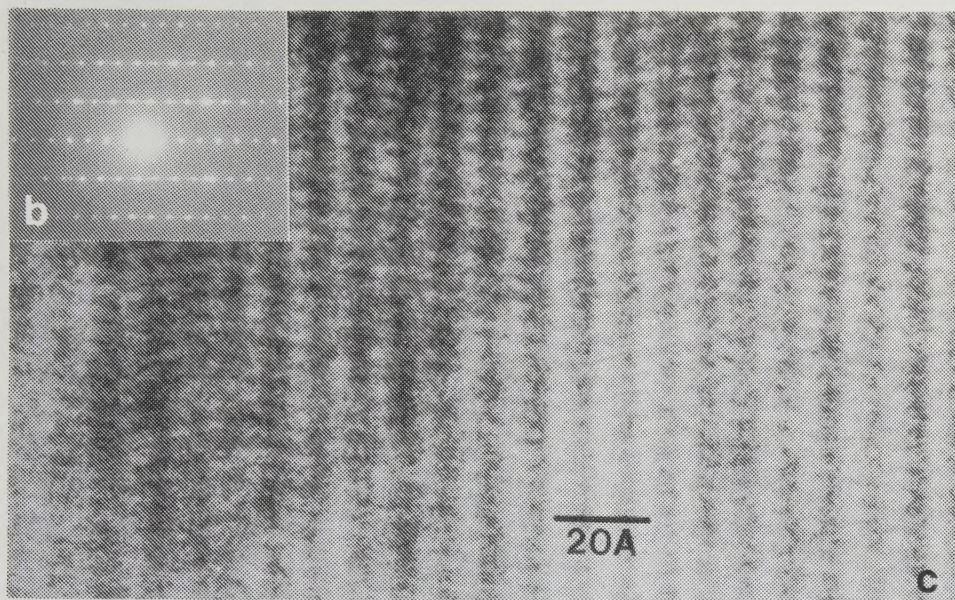


Fig 6b. Electron Diffraction Pattern (EDP) from a μ -phase crystal containing twin defects.

Fig 6c. Lattice image of a Fe-Mo μ -phase crystal. The wavy texture in the image is caused by twin defects.

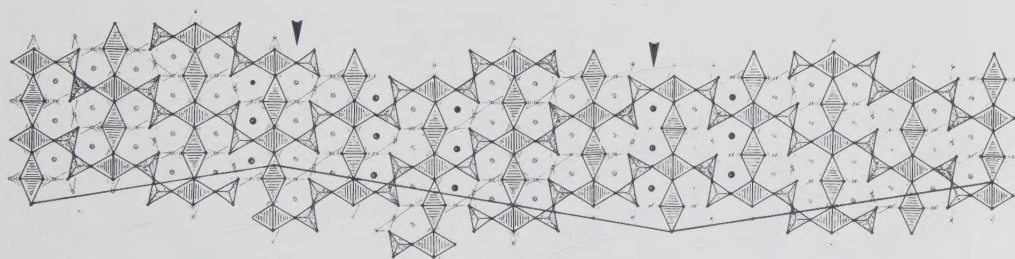


Fig 6d. Structural drawing of the μ -phase where irregular twin operations change the direction of the oblique unit cell.

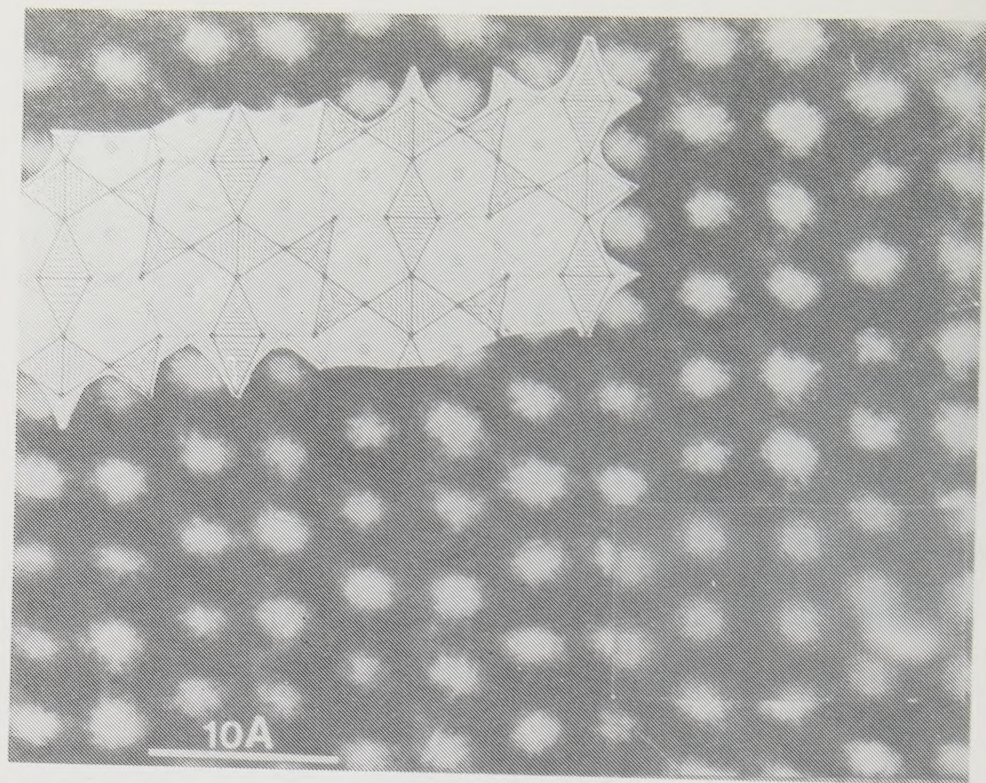


Fig 7a. CSI of a perfect Ni-Cr-Nb μ -phase crystal. Calculated image and structural drawing are inserted to match the CSI (NSLICE = 8, $\Delta f = -600 \text{ \AA}$).

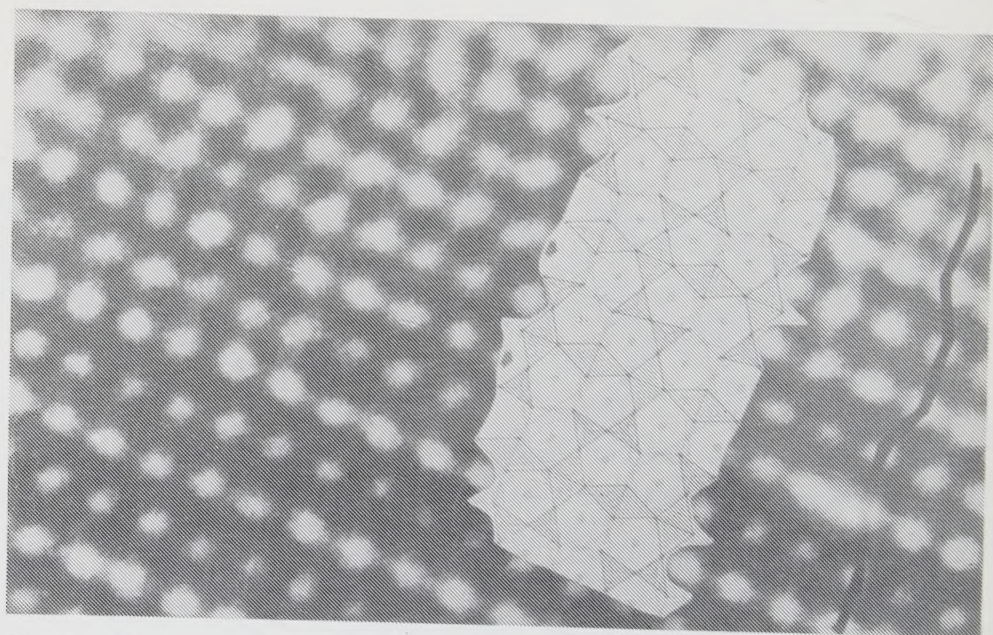


Fig 7b. CSI of a twin defect in a Ni-Cr-Nb μ -phase crystal. Arrows in the inserted structural drawing indicate twin planes.

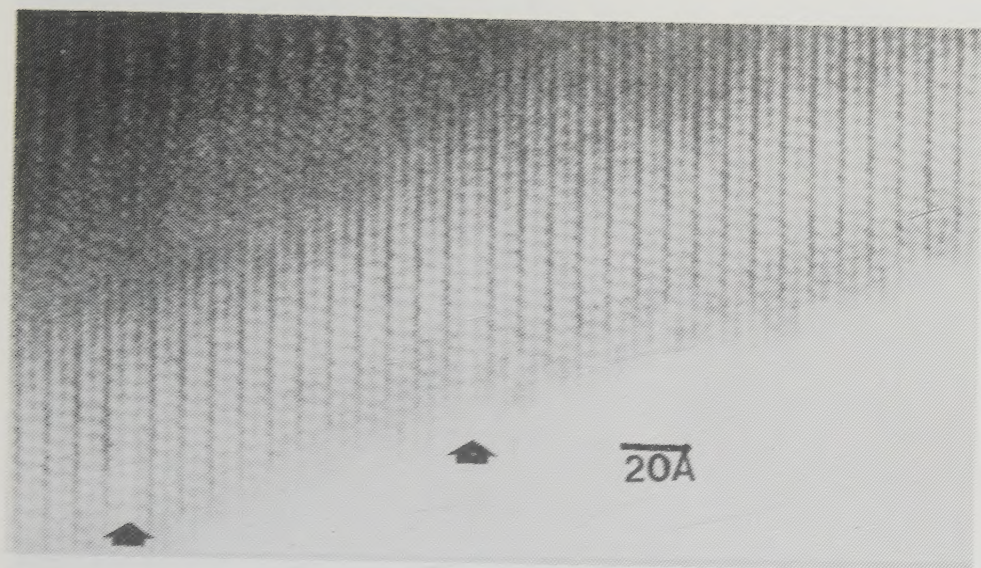


Fig 7c. CSI of a Mo-Co-Si μ -phase crystal. The arrows point at defects that can be explained with an intergrowth of one slab with the Zr_4Al_3 -structure ($3 \times \infty$ white dots).

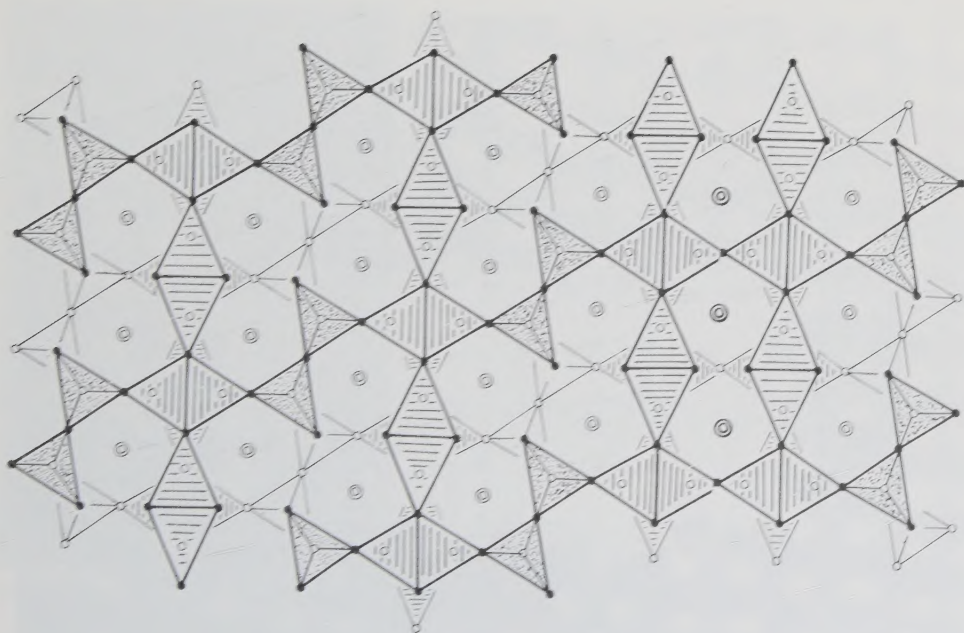


Fig 7d. Drawing of the μ -phase structure with an intergrowth of one slab with the Zr_4Al_3 -structure ($3 \times \infty$ pentagonal antiprisms).

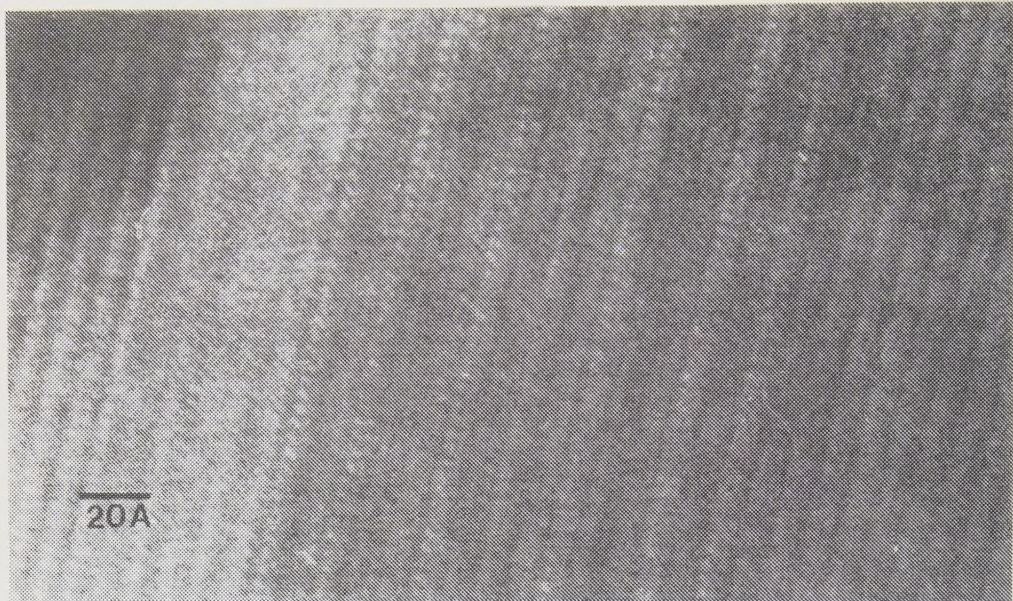


Fig 7e. Lattice image showing planar defects in a Fe-Mo μ -phase crystal. The orthogonality of the defect area suggests an intergrowth of the Zr_4Al_3 - or $MgZn_2$ -structures, but the resolution is too poor to decide which one.

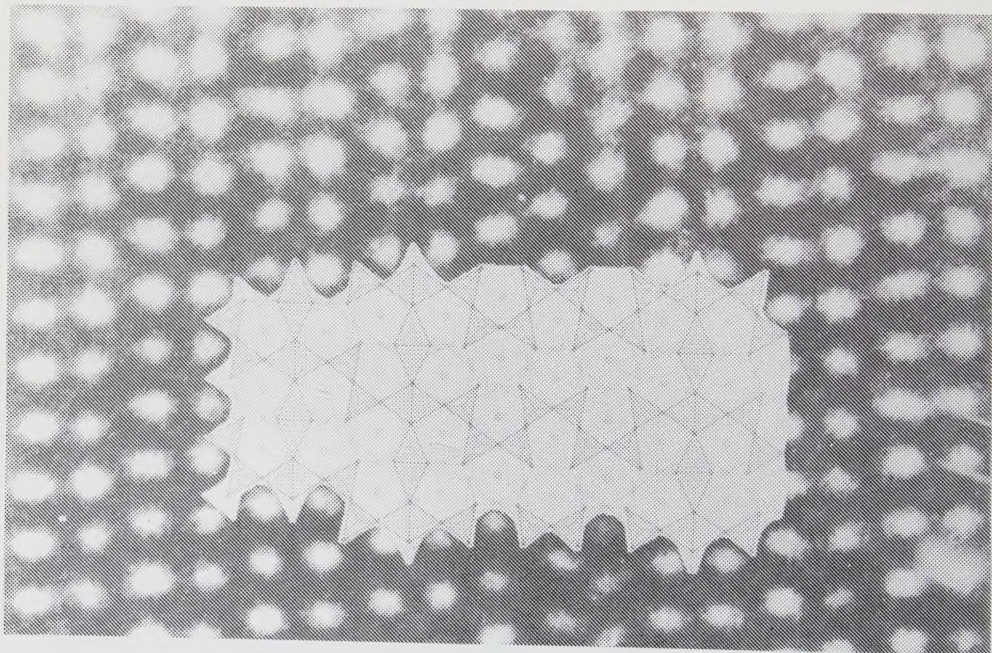


Fig 7f. CSI of a Ni-Cr-Nb μ -phase crystal with an intergrowth defect with the $MgZn_2$ -structure. The white dots represent the position of the atoms centering the pentagonal anti-prisms. The pattern of the white dots in the defect area gives clear evidence of an intergrowth with the $MgZn_2$ -structure at this resolution.

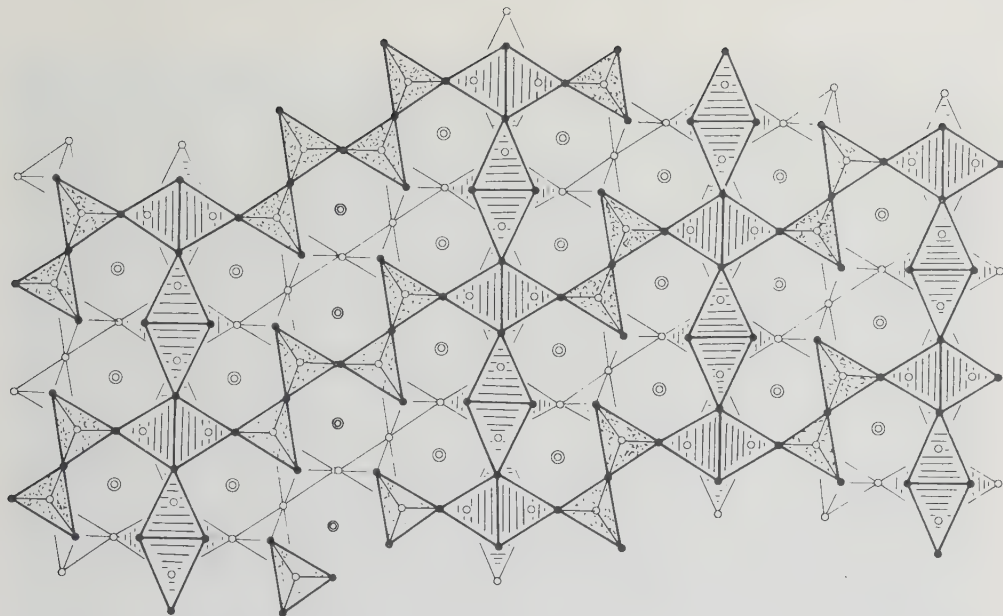


Fig 7g. Structural drawing of the μ -phase with an intergrowth of the MgCu_2 -structure.

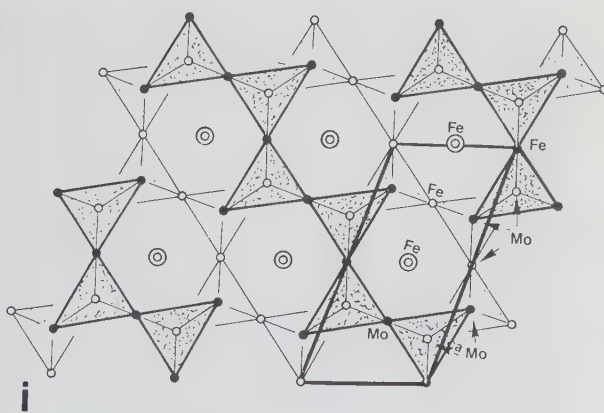
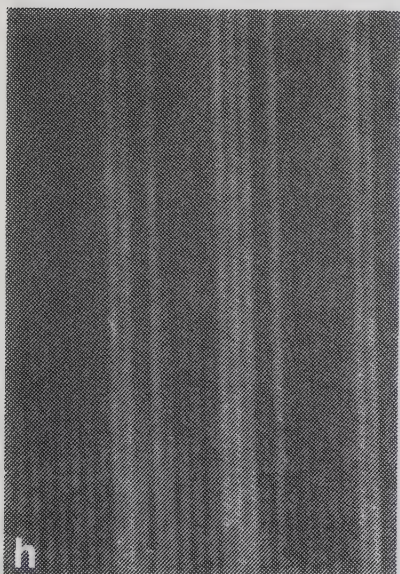
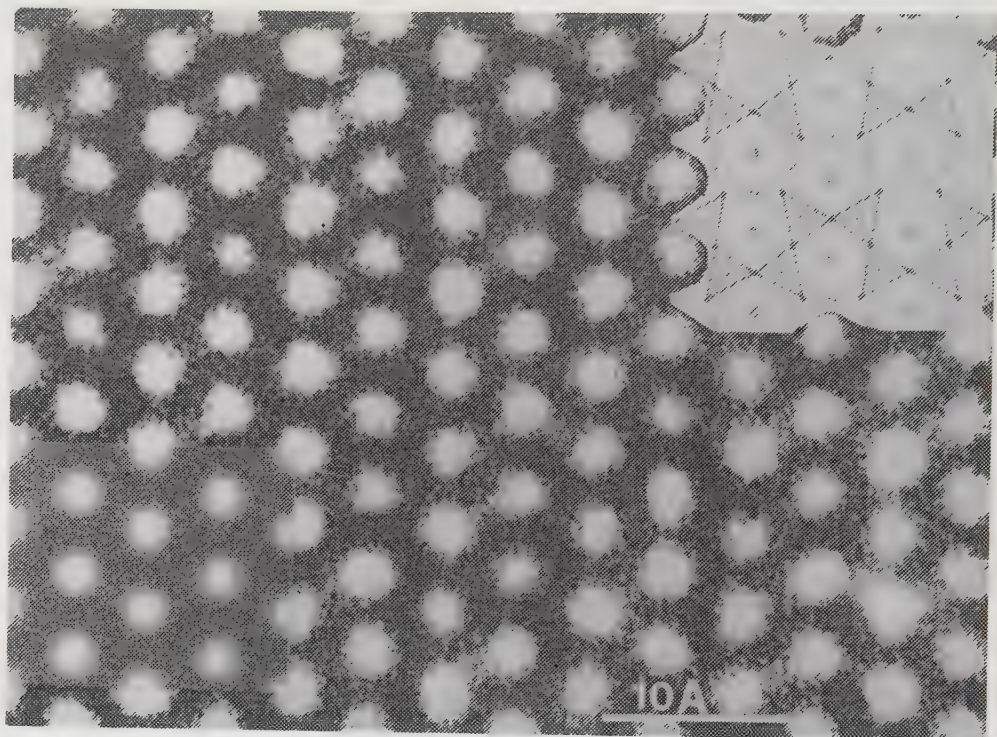
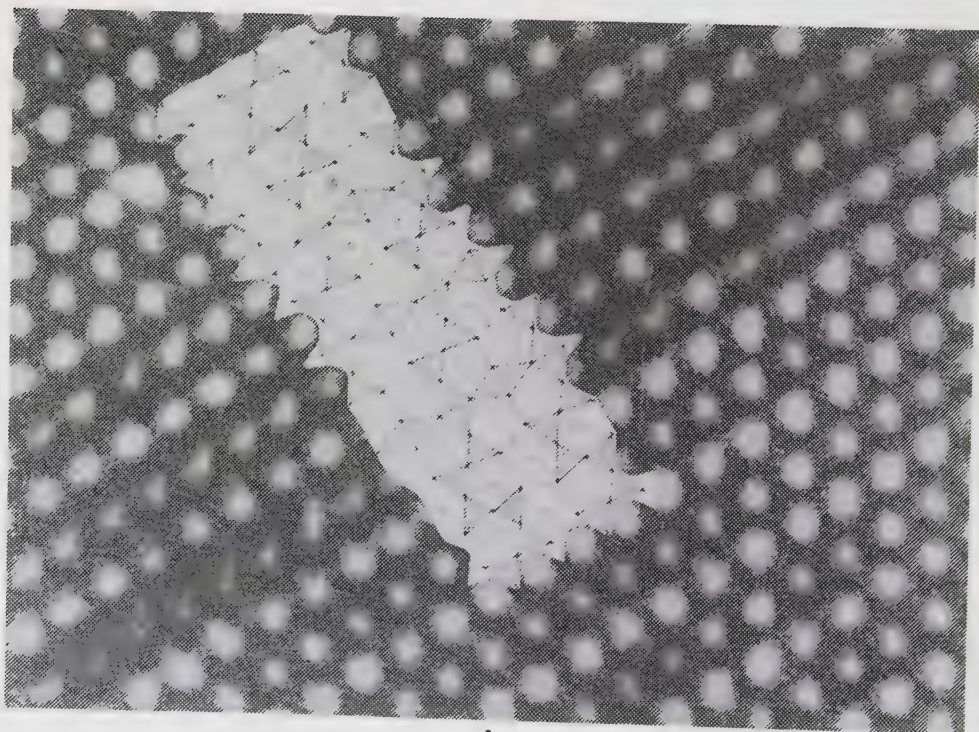


Fig 7h. Lattice image from a Fe-Mo μ -phase crystal with an intergrowth defect with the MgCu_2 -structure. The spacing over the defect is double of what can be expected.

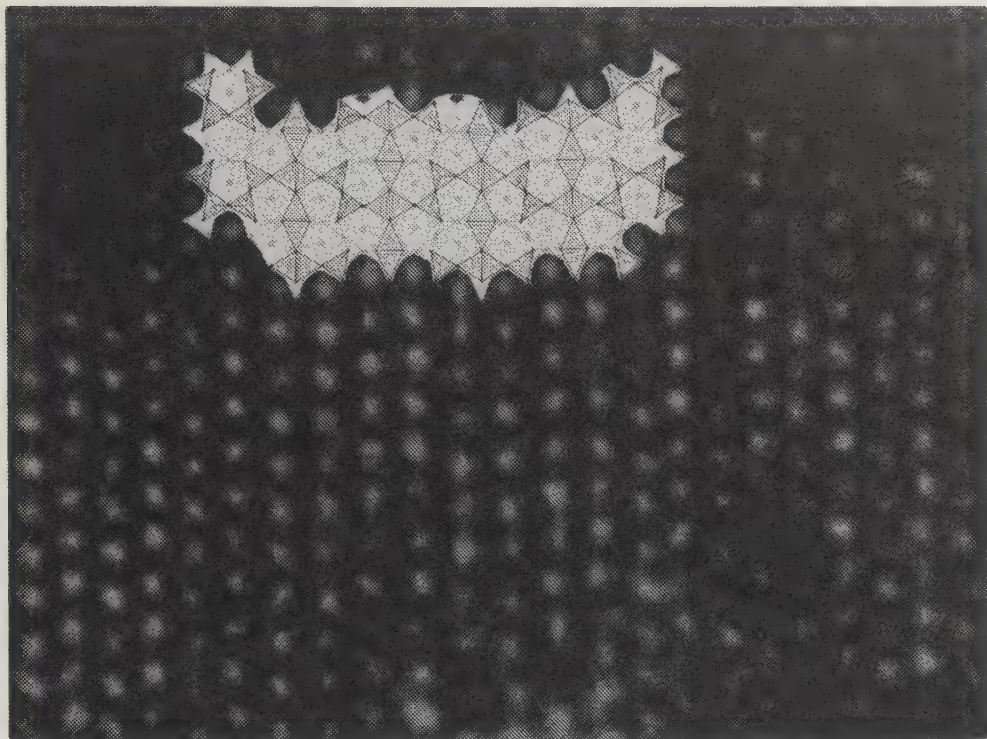
Fig 7i. A suggestion for the ordering of atoms in a Fe-Mo crystal with the MgCu_2 -structure. This gives a doubled repetition unit in the projected cell.



a



b



C

Fig 8a. CSI of a Ni-Cr-Nb crystal with the MgZn_2 -structure. Structural drawing and calculated image are inserted ($\text{NSLICE} = 8$, $\Delta f = -600 \text{ \AA}$).

Fig 8b. CSI of a Ni-Cr-Nb crystal with the MgZn_2 -structure and an intergrowth defect with the μ -phase structure.

Fig 8c. CSI of a Ni-Cr-Nb crystal with the MgZn_2 -structure and an intergrowth defect with the K_7Cs_6 -structure (twinned μ -phase at arrows).

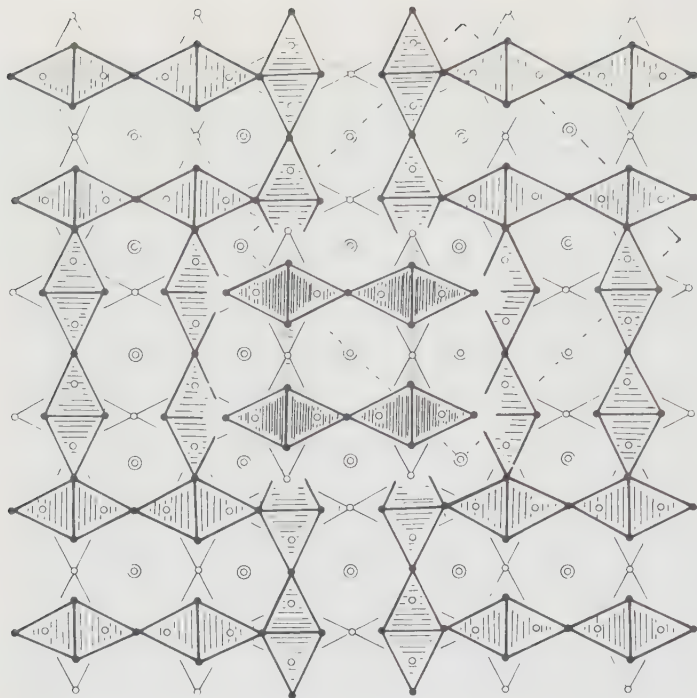


Fig 9a. Drawing of the idealized structure of Mo_3CoSi . A 2×2 Cr_3Si -block is emphasized.

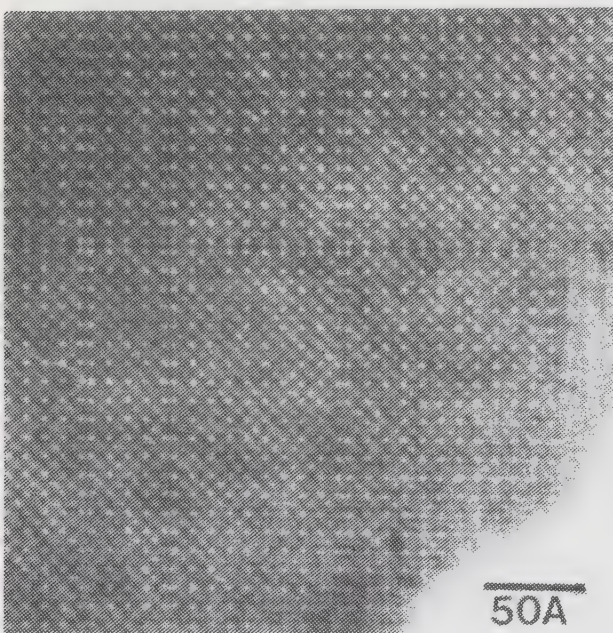


Fig 9b. CSI of a Mo_3CoSi crystal. The atomic arrangement in the defects can be explained with crystallographic shear operations (CS). In the cross-over of two perpendicular defects, where four bright dots form a small square, a piece with the A15-structure is formed. Strong white and greyish dots represent atoms centering hexagonal and square antiprisms respectively.

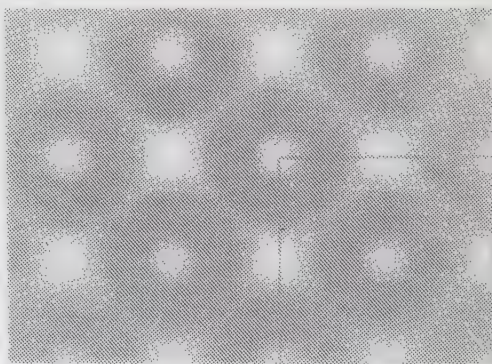


Fig 9c. Calculated image of Mo_3CoSi (NSLICE = 10, $\Delta f = -1000$ Å).

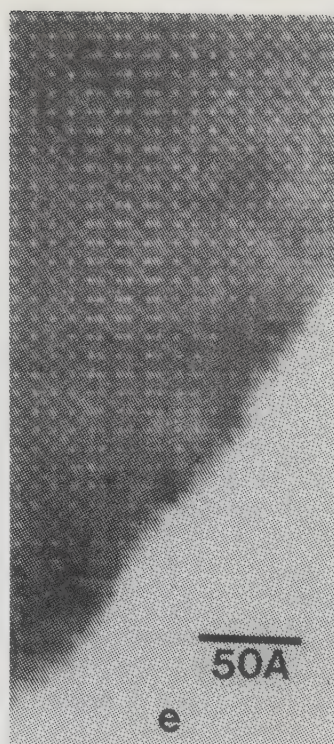
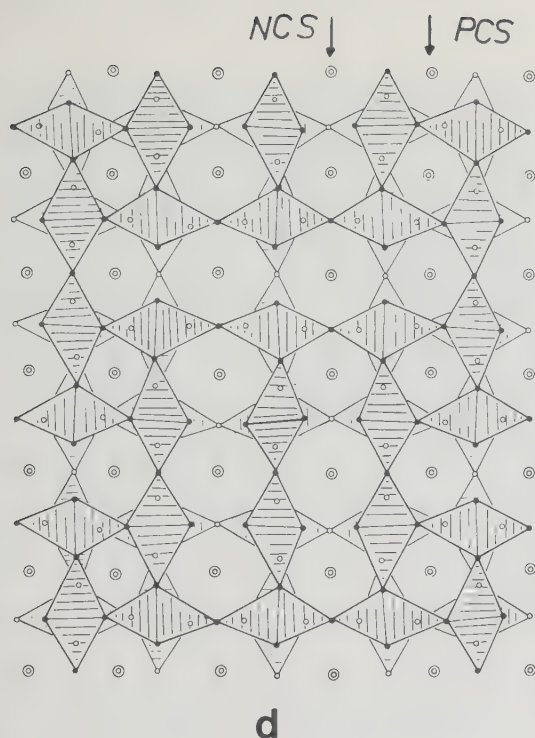


Fig 9d. The atomic arrangement of the defect shown in Fig 9b. Negative and positive CS planes (NCS and PCS) are indicated by arrows. These operations result in two hexagonal antiprisms as neighbours.

Fig 9e. Three parallel CS defects in a Mo_3CoSi crystal.

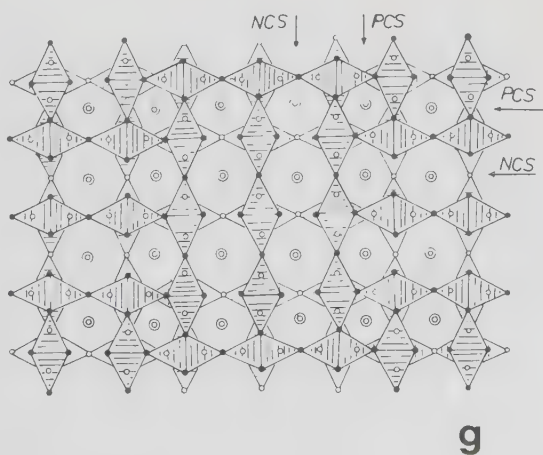
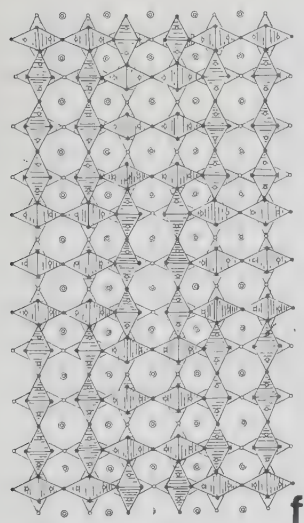


Fig 9f. Structural drawing of a 2×3 Cr_3Si -block structure. This drawing represents the atomic arrangement in Fig 9e.

Fig 9g. Perpendicular CS-operations in the Mo_3CoSi -structure give a piece (3×3) with the A15-structure in the cross-over (see Fig 9b).

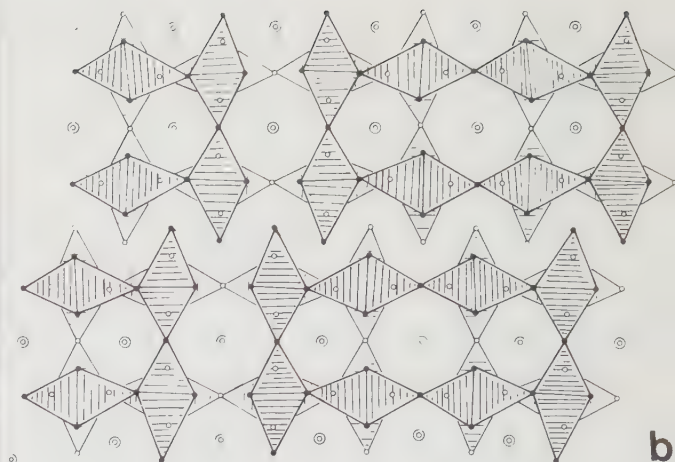
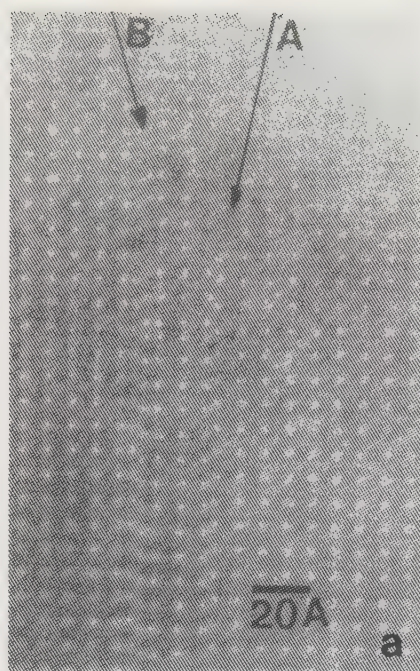


Fig 10a. CSI of a Mo_3CoSi crystal showing two parallel defects of slip type. The defect labelled B is surrounded by two defects of CS-type.

Fig 10b. Drawing of a slip defect in the Mo_3CoSi -structure. The two parts are shifted $\frac{1}{4}C$ with respect to each other.

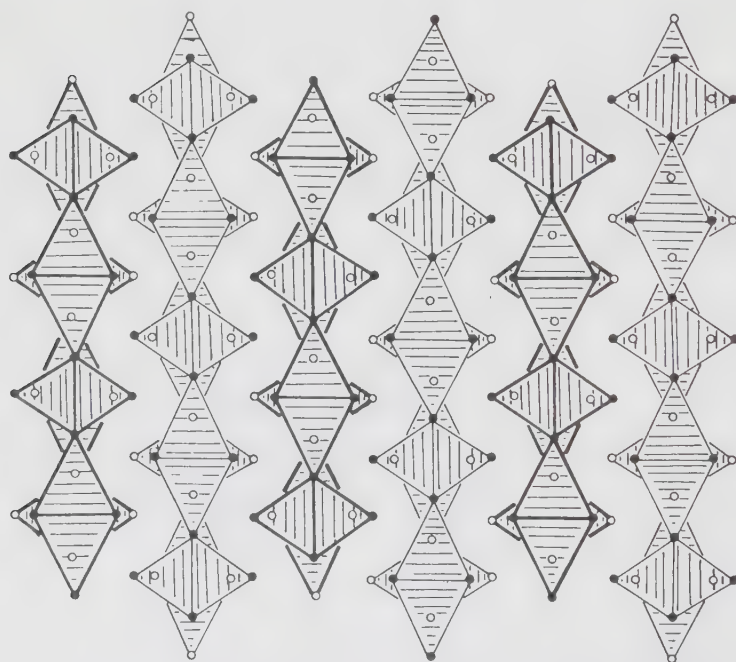


Fig 10c. Structural drawing of Mn_4B . Regular slip operations in this structure result in the Zr_4Al_3 -structure and slip and CS yield the CuAl_2 -structure.

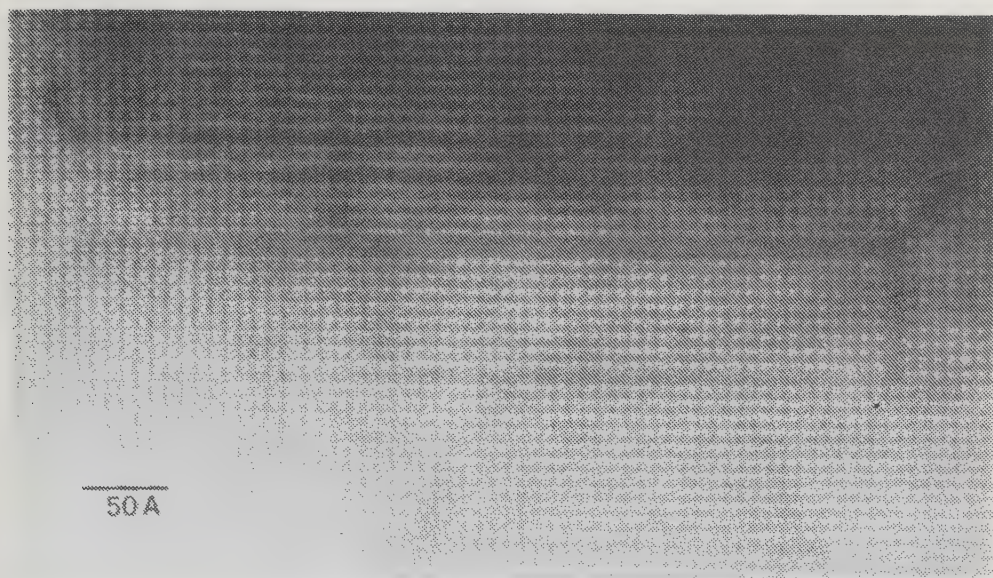


Fig 11a. CSI of a Mo_3CoSi crystal with short slip defects parallel to the a -axis that unite other defects of slip and CS type.

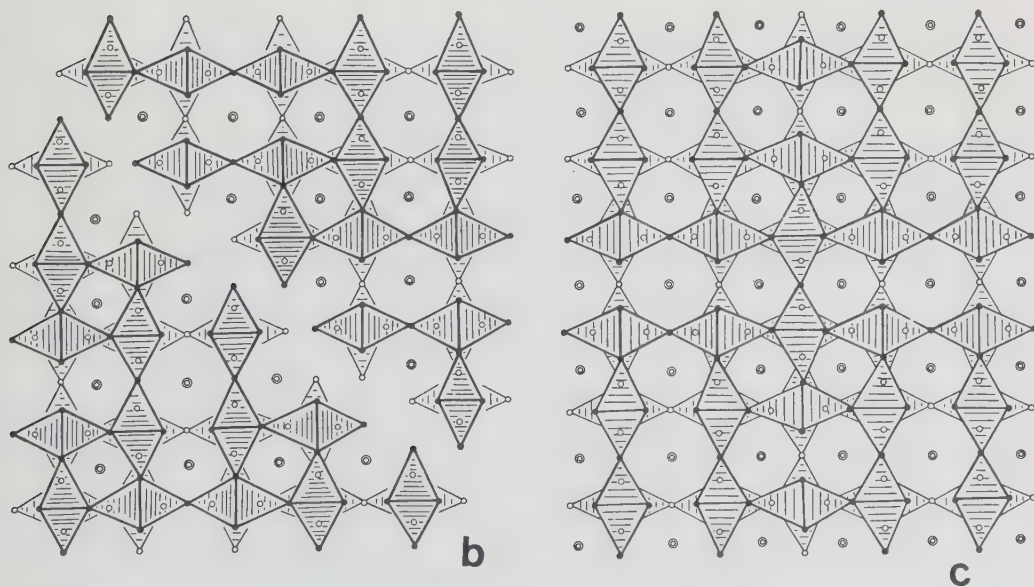


Fig 11b. Atomic arrangement of a short slip defect which agrees with the image of Fig 11a.

Fig 11c. Structural drawing of a PCS defect in the Mo_3CoSi -structure giving two square anti-prisms as neighbours.

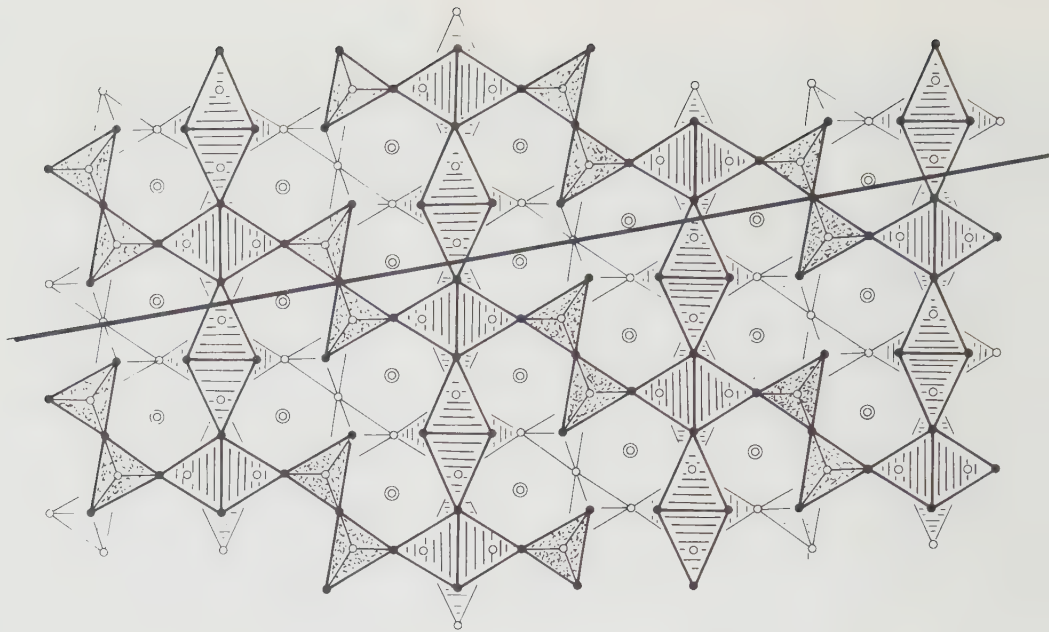


Fig 12a. The μ -phase structure. Twin and slip along the line gives a piece with the M-phase structure.

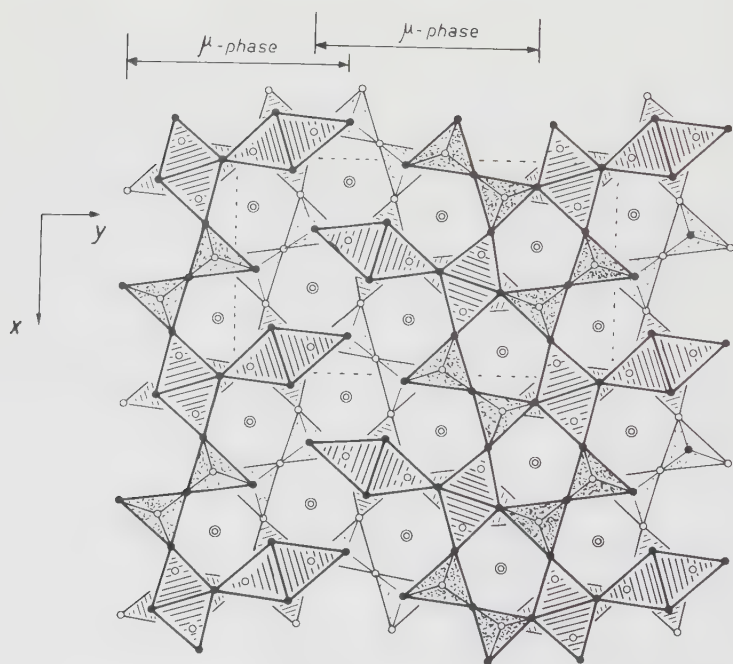


Fig 12b. Structural drawing of the M-phase. The μ -phase parts are indicated.

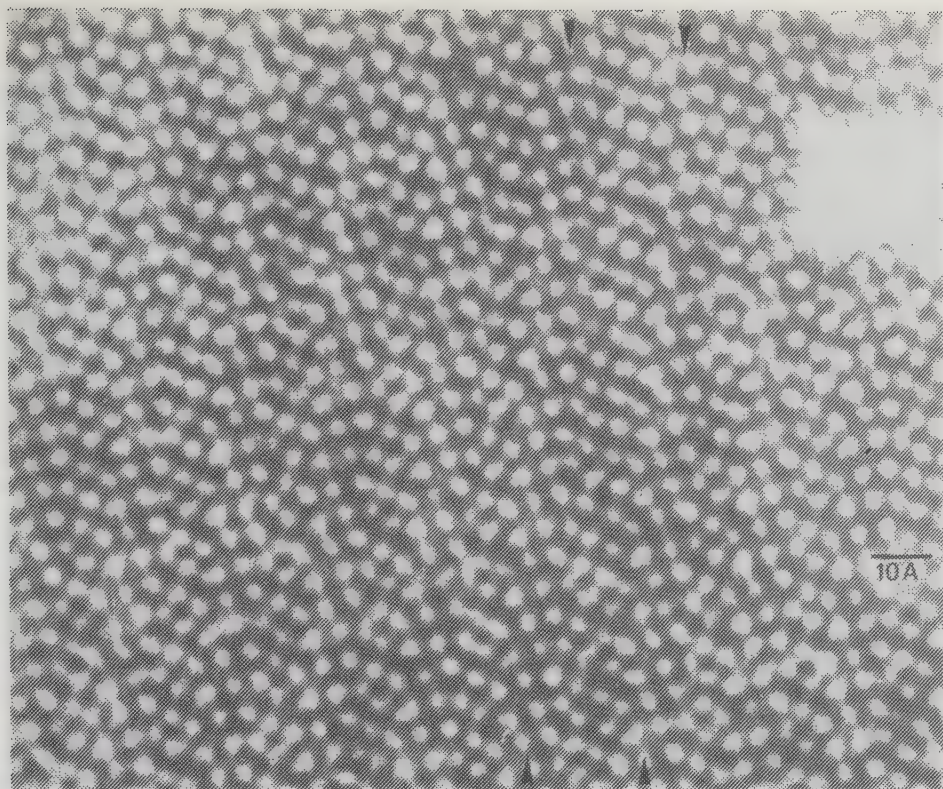


Fig 12c. CSI of an M-phase crystal ($\text{Nb}_{48}\text{Ni}_{39}\text{Al}_{13}$). White dots correspond to atoms centering pentagonal anti-prisms. The arrows frame a defect with an extra long μ -phase part.

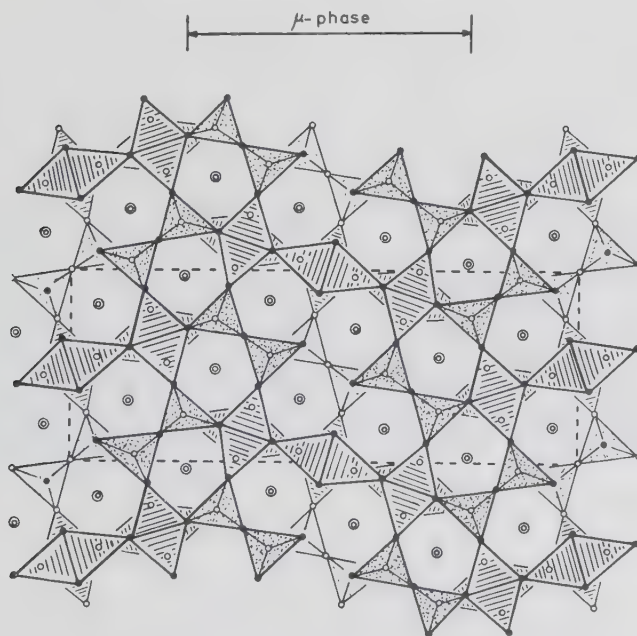


Fig 12d. Structural drawing of the defect in Fig 12c. Dashed lines indicate the unit cell of a hypothetical structure, generated by regular intergrowth of one μ -phase slab in the M-phase structure.

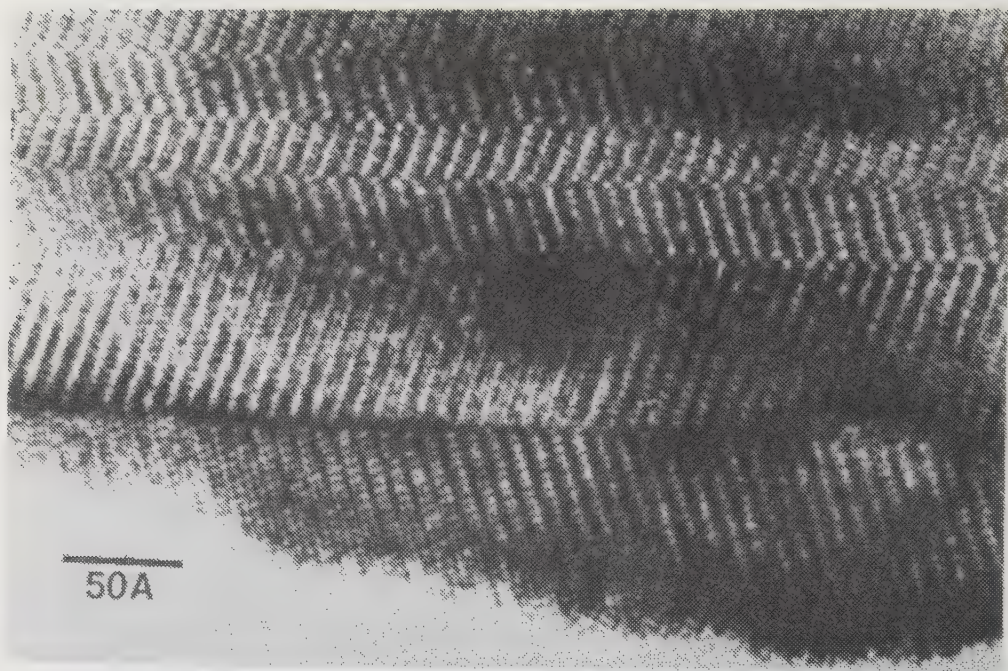
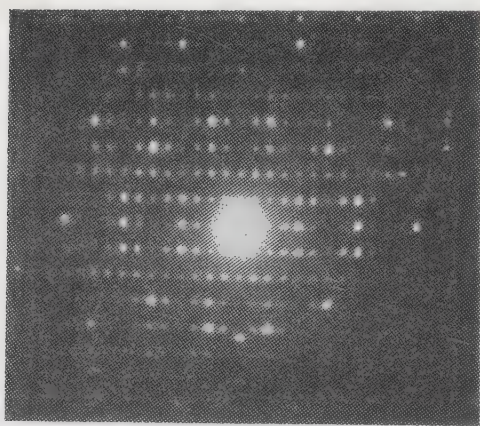
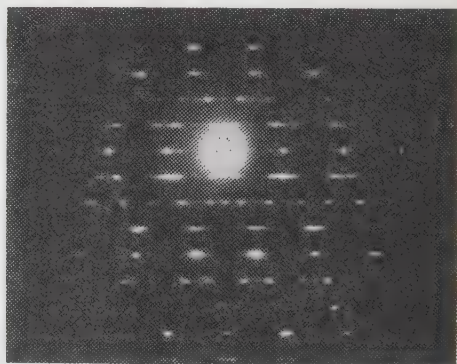


Fig 12e. CSI of an M-phase crystal with large μ -phase structural parts connected as in the M-phase structure.



f



g

Fig 12f. EDP from the same crystal as Figs 12e and g, but from an area dominated by the M-phase structure.

Fig 12g. EDP mainly recorded from the part of the M-phase crystal shown in Fig 12e. Note the resemblance to Fig 6b.



Fig 12h. Micrograph from a partly transformed crystal with M-phase composition. It is clear from this image that the defects are formed in the transformation from bcc to M-phase. The cracks must have been introduced in the grinding process, since the defects continue through the crack despite the fact that the normal interatomic bonds are broken.

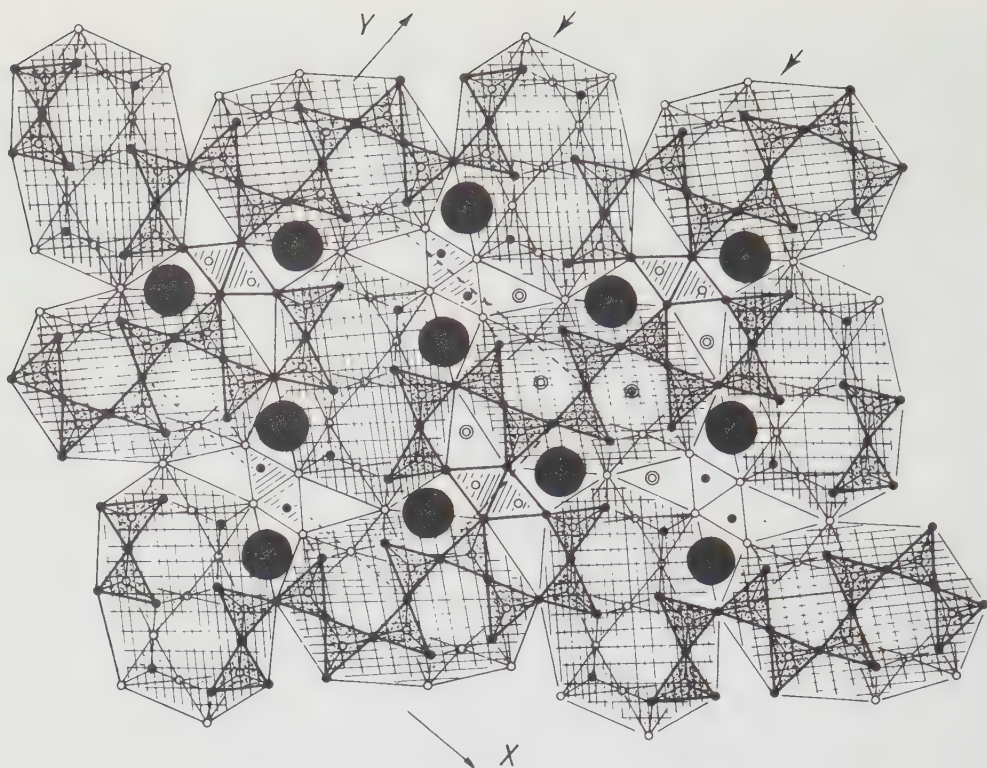


Fig 13a. Structural drawing of the X-phase ($\text{Mn}_{45}\text{Co}_{40}\text{Si}_{15}$). Dashed areas represent fourling units. Black dots show atomic positions giving white contrast in the CSI.

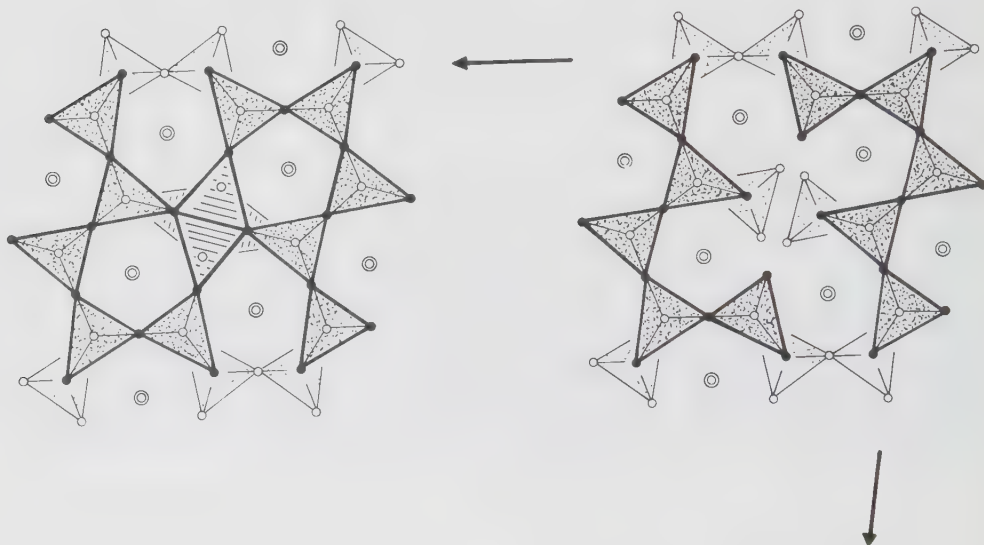


Fig 13b. Generation of a TS by combination of two parts with the MgZn_2 -structure.

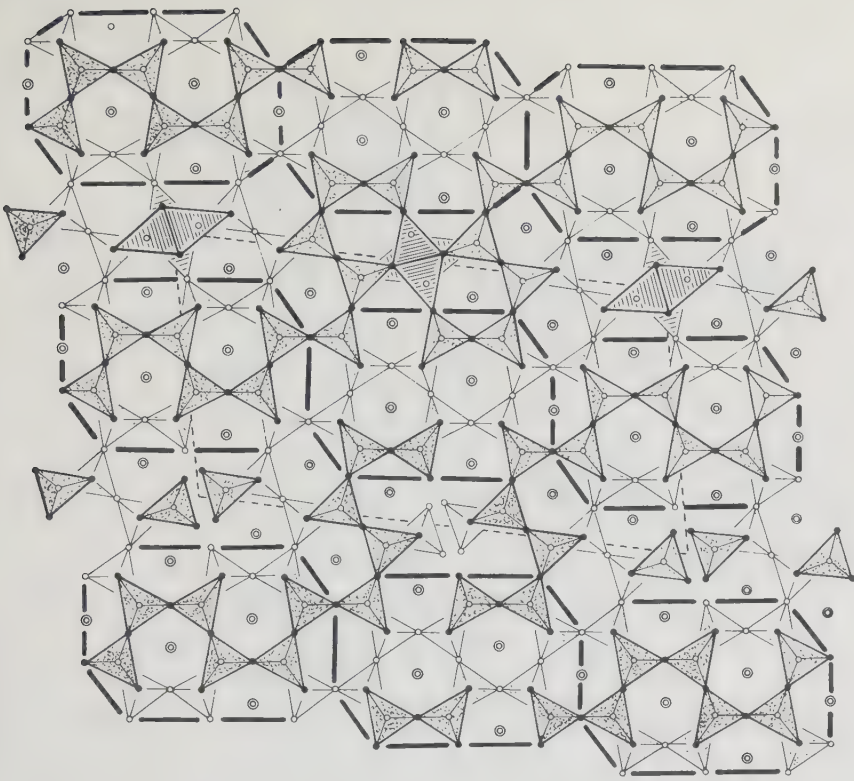


Fig 13c. Structural drawing of Mg_4Zn_7 constructed with $MgZn_2$ -parts. These can be varied in size to give different intervals between the generated TS's.

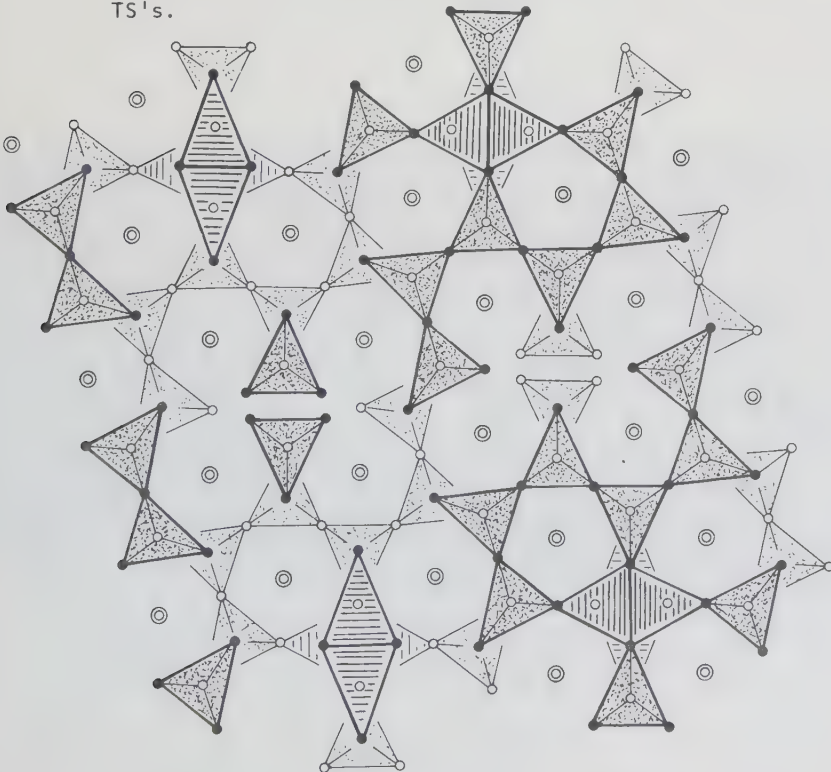


Fig 13d. Structural drawing of $(Co_{0.57}Si_{0.43})_3V_2$ constructed with $MgZn_2$ -parts.

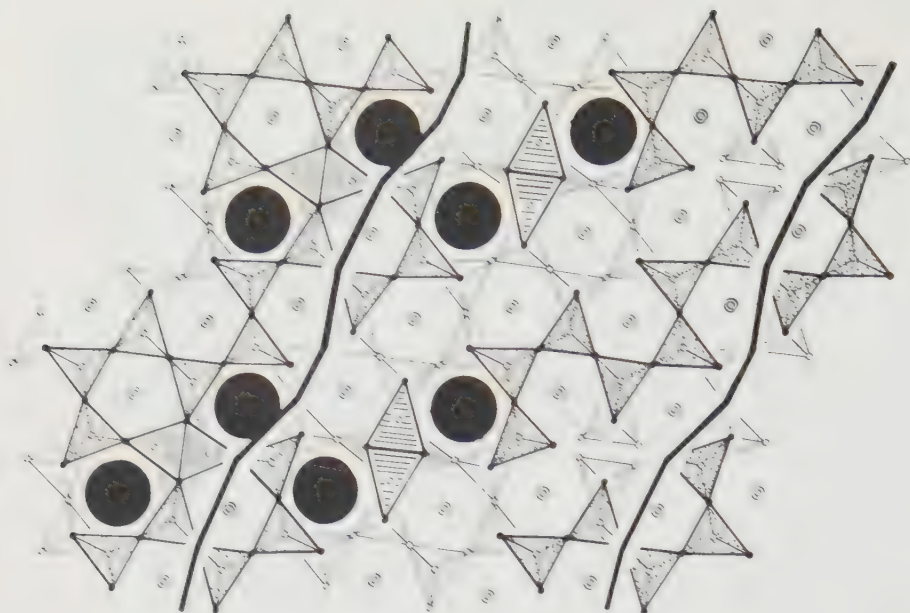


Fig 13e. Structural drawing of a hypothetical structure constructed with MgZn_2 -parts (calculated composition $\text{Mg}_{45}\text{Zn}_{55}$). This structure is also generated if regular chemical twin and slip operations are applied to the structure of the X-phase (along the short arrows in Fig 13a). The black dots indicate the atomic positions giving white contrast in the CSI.

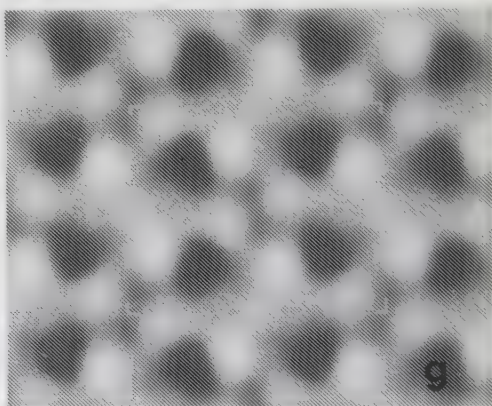
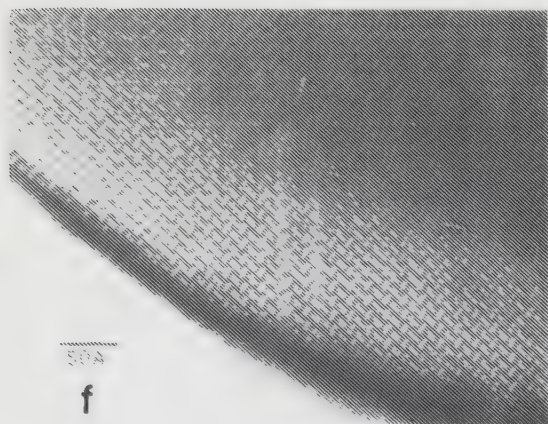


Fig 13f. CSI of an X-phase crystal. The defects run parallel to the y-axis and their structure can be derived with chemical twin operations.

Fig 13g. Calculated image of the X-phase. Corners of the unit cell are indicated (NSLICE = 20, $\Delta f = -1150$ Å).

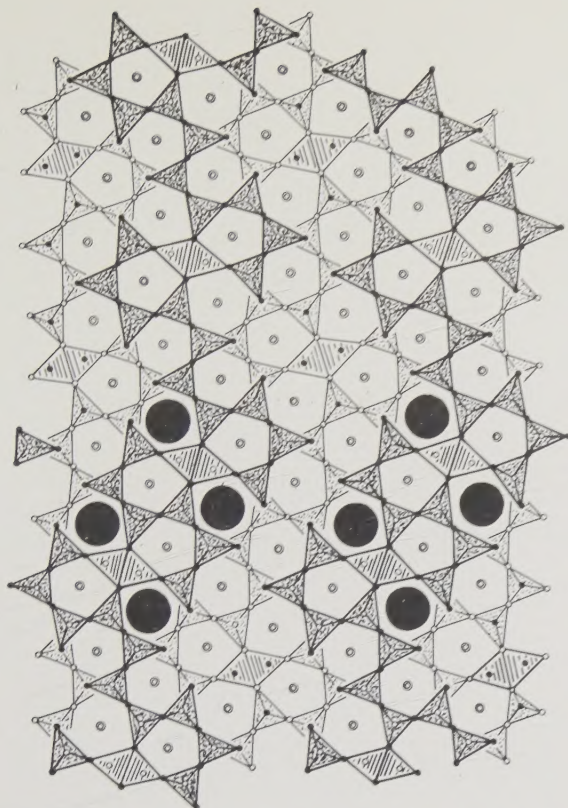


Fig 13h. Structural drawing where a chemical twin and slip operation have been carried out along the x-axis in the X-phase structure. Black dots indicate atomic positions generating white contrast in the CSI.

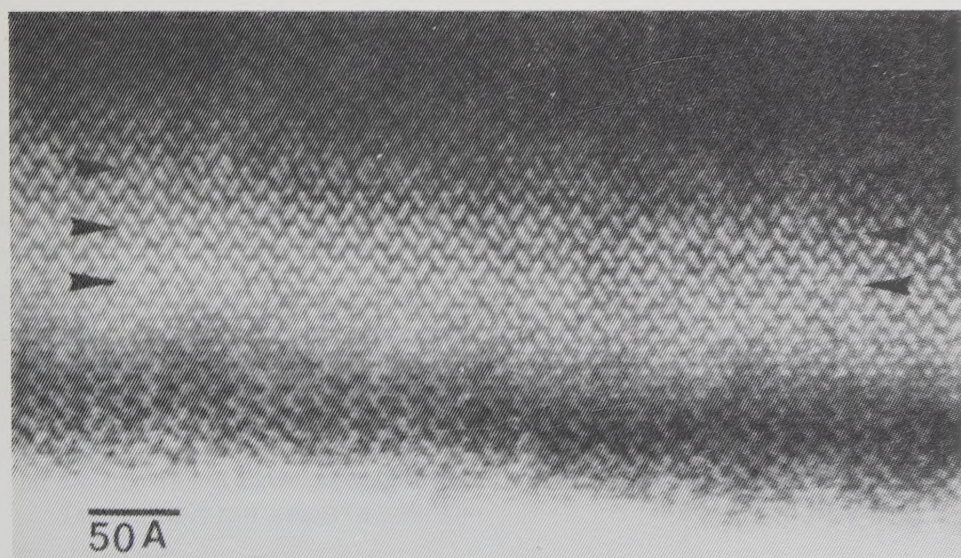


Fig 13i. CSI of an X-phase crystal with three twin defects (see arrows) running parallel to the x-axis.

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